Simulating Electron Cooling Physics with VORPAL – Status, Current Plans & Future Developments

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Outline

- Status of the Current Phase II SBIR Project at Tech-X
- Plans for the remainder of the Phase II
- Ideas for future work

Motivation & Goals of Current Phase II Project

- Motivation
  - Support R&D at BNL to help understand and optimize potential performance of the proposed electron cooling section for RHIC
- Primary goal
  - Develop first-principles capability to model electron cooling physics for relativistic ions, especially for RHIC parameters
- General Approach
  - Follow the galactic dynamics community – use direct Coulomb field solve with variable time-stepping to resolve close collisions
  - Accurately calculate friction and diffusion coefficients for the ions
    - » Resolve differences in analytical calculations
      - *Coulomb log >> 1; uniform e- distribution (no space charge)*
    - » Determine validity of Z^2 scaling
    - » Understand the effects of beam space charge on friction
    - » Understand the effects of magnetization
      - *from weak to strong; effect of field errors*
    - » What happens for Coulomb log of order unity or smaller?
    - » For one set of parameters, provide table of coefficients to BetaCool, SimCool

Current Status - Overview

- Friction coefficients for electron cooling are being simulated at Tech-X and BNL using the VORPAL code
- Some caveats:
  - We are currently neglecting e-/e- interactions
    - » Not too bad, because the interaction time is short
    - » Initial work with a Poisson solver to correctly capture the e-/e- interactions and the Debye shielding has begun
  - The ion is also influenced by large-scale space charge forces
    - » Until recently, this effect was removed from the friction force that we extract from the simulation data as follows:
      - *Run Au+79 ion and "anti" ion (opposite sign)*
      - *Average the velocity changes (space charge effects cancel out, leaving friction)*
  - Recently developed approach to remove bulk space charge forces
    - » When calculating forces on any one particle, temporarily shift far away particles from top-to-bottom (or vice-versa), left-to-right, etc. so that each particle is effectively in the center of the distribution

4^{th}-Order Predictor/Corrector Hermite Algorithm

- Algorithm developed and used extensively by galactic dynamics community
  - J. Makino, The Astrophysical Journal **369**, 200 (1991)
  - J. Makino & S.J. Aarseth, Publ. Astron. Soc. Japan **44**, 141 (1992)
- The predictor step looks like this:

$$\mathbf{v}_{p,j} = \frac{1}{2}\left(t - t_j\right)^2 \dot{\mathbf{a}}_j + \left(t - t_j\right)\mathbf{a}_j + \mathbf{v}_j$$

$$\mathbf{x}_{p,j} = \frac{1}{6}\left(t - t_j\right)^3 \dot{\mathbf{a}}_j + \frac{1}{2}\left(t - t_j\right)^2 \mathbf{a}_j + \left(t - t_j\right)\mathbf{v}_j + \mathbf{x}_j$$

where

$$\mathbf{a}_i = \frac{q_i}{m_i}\mathbf{v}_i \times \mathbf{B} + \frac{q_i}{4\pi\varepsilon_0 m_i}\sum_j \frac{q_j \mathbf{r}_{ij}}{\left(r_{ij}^2 + r_c^2\right)^{3/2}}$$

$$\mathbf{r}_{ij} = \mathbf{x}_{p,j} - \mathbf{x}_{p,i}$$

$$\mathbf{v}_{ij} = \mathbf{v}_{p,j} - \mathbf{v}_{p,i}$$

$$\dot{\mathbf{a}}_i = \frac{q_i}{m_i}\mathbf{a}_i \times \mathbf{B} + \frac{q_i}{4\pi\varepsilon_0 m_i}\sum_j q_j \left[\frac{\mathbf{v}_{ij}}{\left(r_{ij}^2 + r_c^2\right)^{3/2}} + \frac{3\left(\mathbf{v}_{ij} \bullet \mathbf{r}_{ij}\right)\mathbf{r}_{ij}}{\left(r_{ij}^2 + r_c^2\right)^{5/2}}\right]$$

$r_c \to 0$ “cloud” radius

Hermite Algorithm -- continued

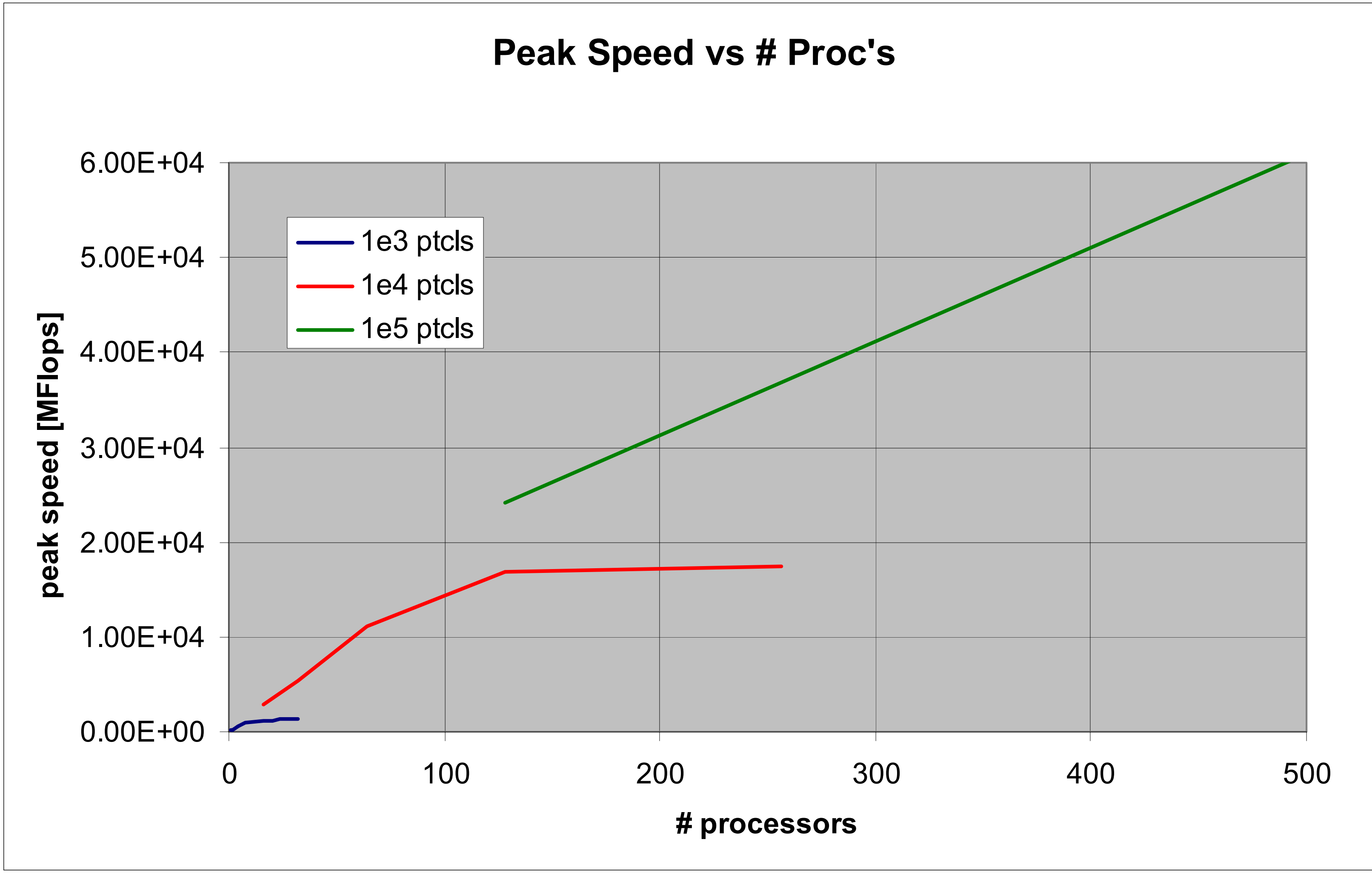
- The corrector step looks like this:

$$\mathbf{x}_i(t_i+\Delta t_i)=\mathbf{x}_{p,i}+\frac{1}{24}\Delta t_i{}^4\mathbf{a}_{0,i}^{(2)}+\frac{1}{120}\Delta t_i{}^5\mathbf{a}_{0,i}^{(3)} \qquad \mathbf{v}_i(t_i+\Delta t_i)=\mathbf{v}_{p,i}+\frac{1}{6}\Delta t_i{}^3\mathbf{a}_{0,i}^{(2)}+\frac{1}{24}\Delta t_i{}^4\mathbf{a}_{0,i}^{(3)}$$

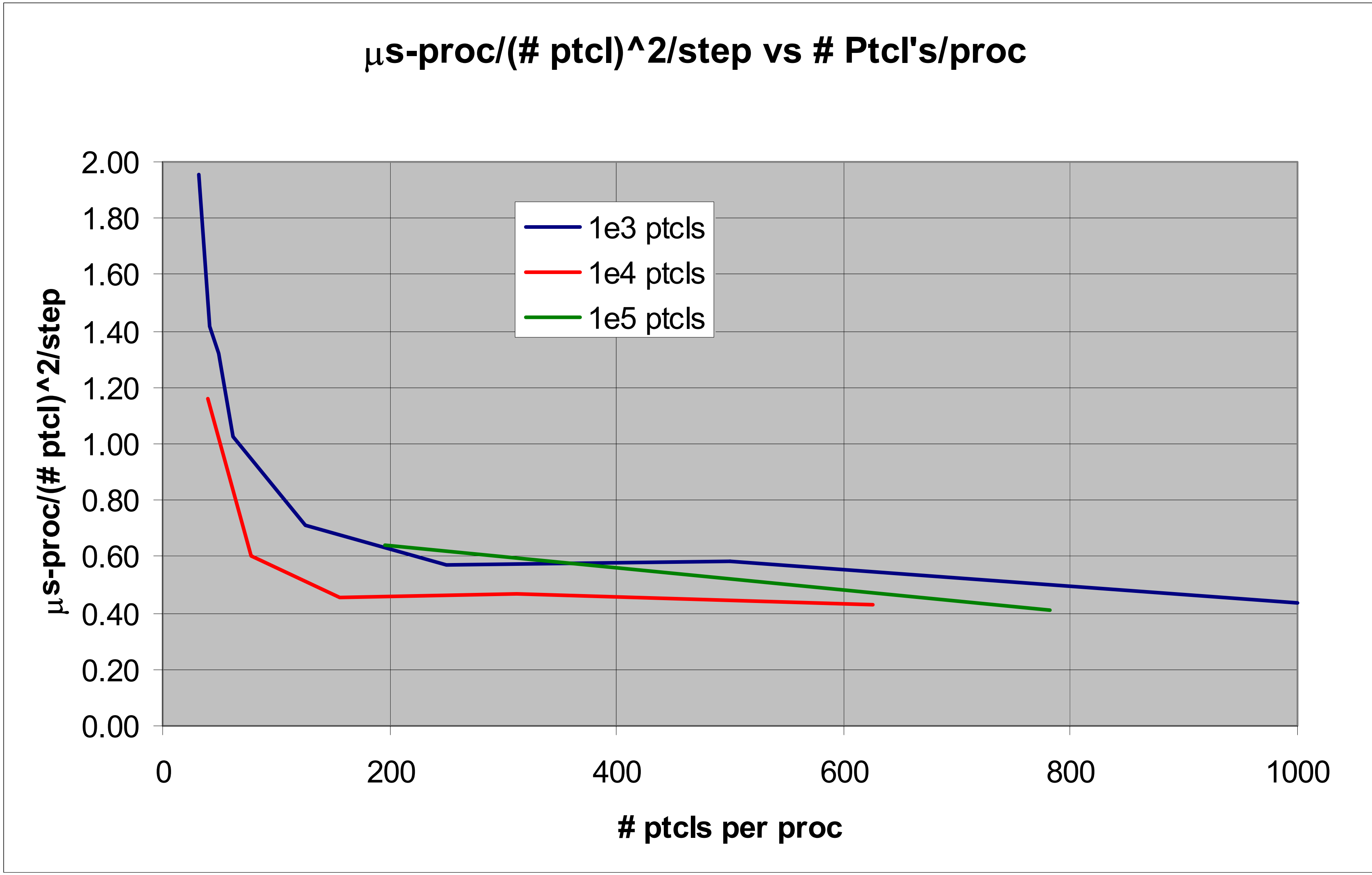
where $\mathbf{a}_{0,i}^{(2)}$ and $\mathbf{a}_{0,i}^{(3)}$ are linear functions of $\mathbf{a}(t)$ and $\dot{\mathbf{a}}(t)$ evaluated at times t_i and $t_i+\Delta t_i$

- Introduction of a magnetic field breaks the 4^{th}-order scaling, unless
  - $\mathbf{B}(\mathbf{x})$ is evaluated again at the predicted positions
  - For the magnetic term in the velocity correction (far right term above):
    - » $\mathbf{a}_{0,i}^{(3)}$ is split into self-field $\mathbf{a}_{self-field,i}^{(3)}$ and magnetic $\mathbf{a}_{magnetic,i}^{(3)}$ terms
    - » the coefficient in front of $\mathbf{a}_{magnetic,i}^{(3)}$ is changed from 1/24 to 5/72
- *Generalization of this algorithm from gravitating masses to ions and magnetized electrons is an important accomplishment*

Good Scaling Demonstrated with up to 512 Processors



200 Particles/Processor is Required for Good Scaling



Single ion dynamics, neglecting e-/e- interactions

- Added the ability to ignore interactions between specified sets of particles
  - Yields an $O(N_{ion}*N_e)$ algorithm (orders of magnitude faster)
    - » Rather than $O(N^2)$, where $N=N_{ion}+N_e$
  - Physically reasonable for $\tau < \omega_{pe}$
    - » Breaks down for longer interaction times or higher e- densities
  - This only works in serial, but parallel version is now underway
  - Can be used with many ions
- We have implemented the ability to include e-/e- interactions via electrostatic PIC
  - Should recover correct shielding
  - Electrostatic PIC algorithm works very well in parallel
  - Combination of Hermite algorithm with PIC is still being tested
- Use of the full $O(N^2)$ Hermite algorithm will be of interest for high-current e- beams
  - Here, e-/e- scattering can break the magnetization

Parallel Boundary Conditions for the Field Solve

- Ewald sums can be used to impose periodic BC's on a Coulomb field solve
  - Early work requires cubic 3D region with periodicity in all dim's
    - » Not very useful for our problem
  - More recent work presents algorithms for periodicity along two of the dimensions, or (separate work) along just one dimension
    - » These papers must be studied more carefully
- Dan Abell derived algorithm for periodicity along 1 dim.
  - Implemented in VORPAL for 2^{nd}-order Boris push, but not for the 4^{th}-order Hermite algorithm
- Recently (last week), a very simple numerical scheme was implemented and seems to be working (still being tested)
  - Enables periodic BC's along 1, 2 or 3 dimensions with just a simple change to the input file

Reduced model

- Assumptions
  - Ions are very weakly perturbed during a single interaction
  - Electron-electron collisions are not important
  - Interactions of single electron with multiple ions are "additive"
- Calculate friction & diffusion coefficients as follows:
  - Choose time step to resolve gyromotion of electrons
  - Use leap-frog integrator with fixed time step:
    - » Apply magnetic force to each ion and electron
    - » Sequence of ion-electron binary collisions
  - Regarding treatment of binary collisions
    - » 2-body Coulomb problem is analytic
    - » Most of the calculations have been completed for implementing this in code
    - » Missing space charge forces could be added via PIC
- Benefits of this approach
  - Each time step is $O(N_e * N_{ion})$
  - Number of time steps is $O(20 * N_{gyro})$
  - Same as for present Hermite algorithm, but should be much faster

Plans for the remainder of the Project

- Goal is to accurately calculate friction and diffusion coefficients for Au+79 ions, with RHIC parameters
  - Accurately simulate the physics
  - Develop improved understanding of the physics
  - Produce improved coefficients for BetaCool, SimCool
- Overview of our future plans
  - Complete code development, testing and benchmarking
  - Address key physics issues
  - Make it easier to generate input files, run parameter sweeps
  - Generate relevant coefficients for BetaCool and SimCool

Code Development

- Neglect of e-/e- interactions
  - Finish parallel implementation
  - Finish development of combined PIC/Hermite
- Parallel Boundary Conditions
  - Need to decide on one or more approaches to implement & test
- Should we proceed with development of a reduced model?
- Creation of input files and running parameter sweeps
  - VORPAL parser is not very sophisticated
  - VORPAL input files allow for great generality
    - » Many opportunities for bugs in the input file
  - Python pre-parser exists now, which helps quite a bit
  - We will develop a small Python application for generating accurate input files, based on input of relevant physical/numerical param.'s
  - We will develop a small Python application that takes one input file, sweeps over a specified parameter, and invokes VORPAL

Testing and Benchmarking

- Resolve differences in analytical calculations
  - Coulomb log >> 1; uniform e- distribution (no space charge)
  - Both magnetized and unmagnetized
  - How strong is the diffusive dynamics?
- Determine validity of Z^2 scaling
- Understand the effects of beam space charge on friction
- Understand the effects of magnetization
  - from weak to strong; effect of field errors
    - » What happens for Coulomb log of order unity or smaller?
    - » For one set of parameters, provide table of coefficients to BetaCool, SimCool